

=> s dimethyl succinate/cn  
L1 1 DIMETHYL SUCCINATE/CN

=> s dimethyl glutarate/cn  
L2 1 DIMETHYL GLUTARATE/CN

=> s dimethyl adipate/cn  
L3 1 DIMETHYL ADIPATE/CN

=> s l1 or l2 or l3  
L4 3 L1 OR L2 OR L3

=> s 1-3  
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12897299 3  
L5 2699485 1-3  
(1(W)3)

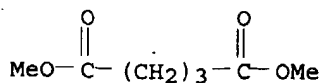
=> \end

\END IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.  
For a list of commands available to you in the current file, enter  
"HELP COMMANDS" at an arrow prompt (=>).

=> d l4 1-3

L4 ANSWER 1 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 1119-40-0 REGISTRY  
CN Pentanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)  
OTHER CA INDEX NAMES:  
CN Glutaric acid, dimethyl ester (6CI, 7CI, 8CI)  
OTHER NAMES:  
CN DBE 5  
CN Dimethyl 1,3-propanedicarboxylate  
CN Dimethyl glutarate  
CN Dimethyl pentanedioate  
CN Methyl glutarate  
CN NSC 58578  
FS 3D CONCORD  
DR 111366-62-2  
MF C7 H12 O4  
CI COM  
LC STN Files: ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, CA, CANCERLIT,  
CAOLD, CAPLUS, CASREACT, CEN, CHEMCATS, CHEMLIST, CIN, CSCHM, CSNB,  
DETERM\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS,  
NIOSTIC, PIRA, PROMT, SPECINFO, TOXCENTER, ULIDAT, USPAT2, USPATFULL  
(\*File contains numerically searchable property data)  
Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*  
(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

622 REFERENCES IN FILE CA (1907 TO DATE)  
22 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
623 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
24 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 2 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN  
RN 627-93-0 REGISTRY  
CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Adipic acid, dimethyl ester (6CI, 8CI)

OTHER NAMES:

CN DBE 6

CN **Dimethyl adipate**

CN Dimethyl hexanedioate

CN Methyl adipate

CN NSC 11213

FS 3D CONCORD

DR 111366-61-1

MF C8 H14 O4

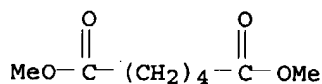
CI COM

LC STN Files: ANABSTR, AQUIRE, BEILSTEIN\*, BIOSIS, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM, CSNB, DETHERM\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PIRA, PROMT, RTECS\*, SPECINFO, TOXCENTER, USPAT2, USPATFULL

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1138 REFERENCES IN FILE CA (1907 TO DATE)

47 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA

1140 REFERENCES IN FILE CAPLUS (1907 TO DATE)

49 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 3 OF 3 REGISTRY COPYRIGHT 2004 ACS on STN

RN 106-65-0 REGISTRY

CN Butanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Succinic acid, dimethyl ester (6CI, 8CI)

OTHER NAMES:

CN DBE 4

CN Dimethyl butanedioate

CN **Dimethyl succinate**

CN Methyl succinate

CN NSC 52209

FS 3D CONCORD

MF C6 H10 O4

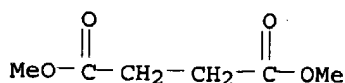
CI COM

LC STN Files: AGRICOLA, ANABSTR, BEILSTEIN\*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMINFORMRX, CHEMLIST, CIN, CSCHM, CSNB, DDFU, DETHERM\*, DIPPR\*, DRUGU, EMBASE, GMELIN\*, HODOC\*, HSDB\*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, NIOSHTIC, PIRA, PROMT, RTECS\*, SPECINFO, SYNTHLINE, TOXCENTER, USPAT2, USPATFULL, VTB

(\*File contains numerically searchable property data)

Other Sources: DSL\*\*, EINECS\*\*, TSCA\*\*

(\*\*Enter CHEMLIST File for up-to-date regulatory information)



\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1343 REFERENCES IN FILE CA (1907 TO DATE)

39 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA  
1344 REFERENCES IN FILE CAPLUS (1907 TO DATE)  
44 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> s 1119-40-0/prep  
'PREP' IS NOT A VALID FIELD CODE  
L6 0 1119-40-0/PREP

=> file caplus	SINCE FILE	TOTAL
COST IN U.S. DOLLARS	ENTRY	SESSION
FULL ESTIMATED COST	29.14	29.35

FILE 'CAPLUS' ENTERED AT 16:08:26 ON 17 FEB 2004  
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FILE COVERS 1907 - 17 Feb 2004 VOL 140 ISS 8  
FILE LAST UPDATED: 16 Feb 2004 (20040216/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 1119-40-0/prep  
623 1119-40-0  
3109528 PREP/RL  
L7 78 1119-40-0/PREP  
(1119-40-0 (L) PREP/RL)

=> s 627-93-0/prep  
1140 627-93-0  
3109528 PREP/RL  
L8 226 627-93-0/PREP  
(627-93-0 (L) PREP/RL)

=> s 106-65-0/prep  
1344 106-65-0  
3109528 PREP/RL  
L9 220 106-65-0/PREP  
(106-65-0 (L) PREP/RL)

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MISSING OPERATOR L8 L9  
The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

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L10 421 L7 OR L8 OR L9

=> s caprolactam and l10  
18908 CAPROLACTAM  
L11 4 CAPROLACTAM AND L10

=> s l11 AND WASTE AND, ALKALINE  
334409 WASTE

103807 ALKALINE  
L12 0 L11 AND WASTE AND ALKALINE

=> s l11 AND NITRIC ACID  
141652 NITRIC  
3779532 ACID  
56329 NITRIC ACID  
(NITRIC(W)ACID)

L13 1 L11 AND NITRIC ACID

=> s l11 AND NITRIC ACID AND DECOMP?  
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3779532 ACID  
56329 NITRIC ACID  
(NITRIC(W)ACID)

576273 DECOMP?  
L14 1 L11 AND NITRIC ACID AND DECOMP?

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56329 NITRIC ACID  
(NITRIC(W)ACID)

576273 DECOMP?  
112407 DISTIL?  
L15 1 L11 AND NITRIC ACID AND DECOMP? AND DISTIL?

=> D L11 1-4 IBIB ABS HITSTR

L11 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:376877 CAPLUS

DOCUMENT NUMBER: 138:369025

TITLE: Preparation of bidentate ligands for use in palladium  
catalyzed carbonylation of ethylenically or  
acetylenically unsaturated compounds

INVENTOR(S): Drent, Eit; Van Ginkel, Roelof; Van der Made, Renata  
Helena

PATENT ASSIGNEE(S): Shell Internationale Research Maatschappij BV, Neth.

SOURCE: PCT Int. Appl., 23 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040159	A2	20030515	WO 2002-EP12380	20021105
WO 2003040159	C1	20030731		
WO 2003040159	A3	20040108		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,  
CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,  
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,  
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,  
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ,  
UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU,  
TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,  
CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,  
PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR,  
NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-348205P P 20011109  
EP 2002-77923 A 20020718

OTHER SOURCE(S): CASREACT 138:369025; MARPAT 138:369025

AB Bidentate ligands, R1R2M1-R-M2R3R4, (wherein M1, M2, independently = P,  
As, Sb; R1, R2, R3, R4, independently = substituted organic group and at  
least one of R1, R2, R3 and R4 contains a tertiary carbon atom through  
which the group is linked to M1 or M2; R = bridging group based on a  
trimethylene group connecting M1 and M2 of which the middle carbon atom is

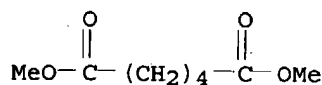
double bonded to a non-metal element chosen from group 14, 15 or 16 of the periodic table of elements) were prepared. For example, di-tert-butylphosphine is reacted with 3-chloro-2-chloromethyl-1-propene to give the corresponding bisphosphonium salt, which is treated with NaOH to give 66% 3-(di-tert-butylphosphino)-2-(di-tert-butylphosphinomethyl)-1-propene, (dtbpm). The prepared compds. are ligands in the palladium catalyzed carbonylation of ethylenically or acetylenically unsatd. compds. For example, 3-pentenitrile undergoes carbonylation in the presence of dtbpm and Pd(OAc)<sub>2</sub> to give the corresponding linear 5-cyanovaleric ester.

IT 627-93-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of bidentate ligands for use in palladium catalyzed carbonylation of ethylenically or acetylenically unsatd. compds., and subsequent reactivity of products of carbonylation)

RN 627-93-0 CAPLUS

CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:146493 CAPLUS

DOCUMENT NUMBER: 138:187402

TITLE: Method for preparation of C4-6 dicarboxylic acid esters from alkali waste liquid generated in manufacturing caprolactam

INVENTOR(S): Chou, Hsien-Chun; Wang, Ke-Shun; Wu, Chung-Ru; Liu, Yao Chung; Liu, Yao-Chung

PATENT ASSIGNEE(S): Chunghuahsing Enterprise Co., Ltd., Taiwan

SOURCE: Jpn. Kokai Tokkyo Koho, 12 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003055303	A2	20030226	JP 2001-387321	20011220
US 2003045750	A1	20030306	US 2002-47835	20020114
PRIORITY APPLN. INFO.:			TW 2001-90119851 A	20010814

AB An efficient process for recovering and manufacturing C4-6 dicarboxylic acids and esters thereof from alkali waste liquid generated in manufacturing caprolactam is provided. The process comprises (1) neutralization of the alkali waste liquid generated in manufacturing caprolactam with H<sub>2</sub>SO<sub>4</sub> to adjust the pH, separation of the oil layer from the water layer, and addition of HNO<sub>3</sub> to the oil layer to convert organic substances into dicarboxylic acids and to obtain a solution of dicarboxylic acids, (2) concentration of the above solution to distill low b.p. monocarboxylic acids and HNO<sub>3</sub> in the first stage and concentration and decomposition of residual HNO<sub>3</sub> and nitro compds. in the second stage to obtain a crude concentrate mainly containing C4-6 dicarboxylic acids, (3) two-step esterification involving addition of C1-4 alkyl alcs. to the crude C4-6 dicarboxylic acid concentrate followed by obtaining a semiesterification intermediate product in the first stage and the obtaining a crude dicarboxylic acid ester product in the second stage, and (4) distillation of the crude dicarboxylic acid ester product to obtain a single or a mixture of dicarboxylic acid esters. Thus, an oil layer (120 g) containing formic acid 2.08, acetic acid 2.07, butyric acid 3.19, valeric acid 0.23, caproic acid 3.19, succinic acid 0.08, glutaric acid 0.85, adipic acid 10.15, 6-hydroxyhexanoic acid 15.07, H<sub>2</sub>O 25.62, and others 35.24 weight% (obtained as described in step 1) was added portionwise at 30° over .apprx.20 min to 600 g 30% aqueous HNO<sub>3</sub>, allowed to react at 30° for 30 min, 50° for 1 h, and 70° for 1 h, and concentrated until the temperature reached at 120°, followed by passing steam to drive out HNO<sub>3</sub> from the solution, stopping steam, and concentration of the resulting solution at

140° to obtain a concentrate (61.5 g) containing formic acid 0, acetic acid 0, butyric acid 0, valeric acid 0.29, caproic acid 0, succinic acid 14.27, glutaric acid 27.36, adipic acid 34.03, 6-hydroxyhexanoic acid 0.53, H<sub>2</sub>O 0, NO<sub>3</sub>- 0.045, and others 36.24 weight%. MeOH 100, the crude concentrate 50, and p-toluenesulfonic acid monohydrate 0.5 g were added to a glass flask fitted with a reflux condenser and allowed to react at 80° for 2 h for the first-stage esterification, followed by removing the reflux condenser, distilling residual MeOH and water formed, raising the temperature to 110°, gradually adding 200 g MeOH over 4 h for the second-stage esterification, and distilling unreacted MeOH and H<sub>2</sub>O formed to give crude dicarboxylic acid ester product (53.5 g) containing succinic acid Me ester 14.13, glutaric acid Me ester 27.68, and adipic acid Me ester 32.64 weight%. The crude dicarboxylic acid ester product (50 g) was distilled at 4 Kpa (130 Torr) to collect the distillate at 110-190°. A clear mixture of C4-6 dicarboxylic acid Me ester (35.1 g) of high purity containing succinic acid Me ester 17.93, glutaric acid Me ester 37.58, and adipic acid Me ester 41.61 weight% was obtained.

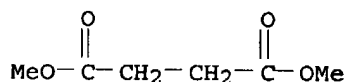
IT 106-65-0P, Succinic acid dimethyl ester 627-93-0P, Adipic acid dimethyl ester 1119-40-0P, Glutaric acid dimethyl ester

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of C4-6 dicarboxylic acid esters from alkali waste liquid generated in manufacturing caprolactam by neutralization, oxidation with nitric acid, concentration, two-stage esterification with alkanols, and distillation)

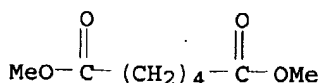
RN 106-65-0 CAPLUS

CN Butanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



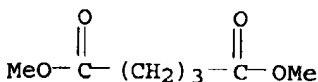
RN 627-93-0 CAPLUS

CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



RN 1119-40-0 CAPLUS

CN Pentanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:43400 CAPLUS

DOCUMENT NUMBER: 84:43400

TITLE: Caprolactam technology. Thermal oxidation of cyclohexanone

AUTHOR(S): Stanek, J.; Capek, A.; Ledvinova, M.

CORPORATE SOURCE: Chemopet. Koncernovy Podnik Spolana, Neratovice, Czech.

SOURCE: Polyamidy '75, Sb. Prednasek (1975), 24-30. Dum Tech. CVTS: Pardubice, Czech.

CODEN: 31WAAO

DOCUMENT TYPE: Conference

LANGUAGE: Czech

AB Acid impurities in tech. cyclohexanone (I) and its oxidation products by air at 100° were determined as Me esters by gas liquid chromatog. and mass

spectra. Me esters and their relative concns. (%) are given for tech. I and its oxidation products: valerate (2.1, 12.6), caproate (9.7, 14.1), 5-hexenoate/4-hexenoate (8.9, 1.9), glutarate (5.5, 13.5), adipate (50, 46.3), and 6-hydroxycaproate (5.8, -). An oxidation scheme was proposed.

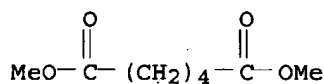
IT 627-93-0P 1119-40-0P

RL: PREP (Preparation)

(by oxidation of cyclohexanone)

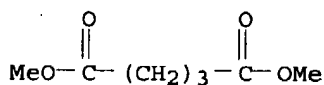
RN 627-93-0 CAPLUS

CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



RN 1119-40-0 CAPLUS

CN Pentanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:463062 CAPLUS

DOCUMENT NUMBER: 75:63062

TITLE: Reprocessing of an aqueous layer, formed during the production of caprolactam, into dimethyl esters of dicarboxylic acids

AUTHOR(S): Freidlin, G. N.; Golubko, L. A.; Glushkova, A. A.; Enyutina, T. M.; Romanova, L. G.; Sapol'kova, G. K.; Samoshina, T. F.; Boyarkin, M. A.

CORPORATE SOURCE: USSR

SOURCE: Khimicheskaya Promyshlennost (Moscow, Russian Federation) (1971), 47(6), 431-3

CODEN: KPRMAW; ISSN: 0023-110X

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The title aqueous layer, containing adipic 21, glutaric 5, and 2 oxalic acids 3%, and smaller amts. of cyclohexanol, cyclohexanone, esters and tar, was oxidized at 2.5 atm in 2 stages at 78-100° with HNO<sub>3</sub>. The H<sub>2</sub>O and HNO<sub>3</sub> were distilled in vacuo to give a melt containing 1.5-3.0% HNO<sub>3</sub> and 97% dicarboxylic acids comprising adipic 19-24, glutaric 42-55, succinic 25-33, and oxalic 0.2-4%. The melt was converted to Me esters at 200° with MeOH in 2 hr in an autoclave. Distillation in vacuo gave the Me esters in 92-4% purity, suitable for plasticizer use.

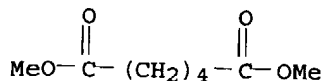
IT 627-93-0P 1119-40-0P

RL: PREP (Preparation)

(recovery of, in caprolactam manufacture)

RN 627-93-0 CAPLUS

CN Hexanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)



RN 1119-40-0 CAPLUS

CN Pentanedioic acid, dimethyl ester (9CI) (CA INDEX NAME)

